4-Hydroxy-1-naphthalenesulfonic acid monosodium salt 6099-57-6 | DTXSID6064113

	6099-	6099-57-6 DTXSID6064113					
Model Performance							
Model		Data					

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 2150 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.80e-01

Confidence level: 6.19e-01

Nearest Neighbors from the Training Set

Image not found

Thiabendazole Measured: 1740 Predicted: 1710 Image not found

Dichlone

Measured: 9550 Predicted: 3350

Image not found

2,7,8,9-Tricyclazole Measured: 1230 Predicted: 242

Image not found

Tetrachlorophthalic acid

Measured: 2000 Predicted: 1980 Image not found

Anilazine
Measured: 1000
Predicted: 1250